CHARGE ORDERING UNDER A MAGNETIC FIELD IN THE EXTENDED HUBBARD MODEL

DUC ANH - LE[1,2], ANH TUAN - HOANG[1] and TOAN THANG - NGUYEN[1]

[1]*Institute of Physics, P.O. Box 429 Bo Ho,*
Hanoi 10 000, Vietnam
[2] *Faculty of Physics, Hanoi University of Education,*
144 Xuan Thuy St, Hanoi, Viet Nam .

Abstract

We study the charge ordering behavior under a magnetic field H in the extended Hubbard model within the coherent potential approximation. At quarter filling, for small H we find that the relative variation of critical temperature is quadratic with the coefficient α smaller than the one for conventional spin-Peierls systems. For intermediate field, a melting of the charge ordering on decreasing temperature under fixed H at various band filling is found.

1. Introduction

After the discovery of a low temperature spin-gapped phase in α'-NaV$_2$O$_5$[1], this compound has attracted a great deal of interest as the second example of an inorganic spin-Peierls material, even with a significantly higher transition temperature than observed for CuGeO$_3$. The properties of NaV$_2$O$_5$, however, have proven to be quite controversial. A number of recent experiments do not conform to current understanding of an ordinary spin- Peierls system[2,3]. In particular, recent NMR measurements revealed the appearance of two inequivalent types of V sites, V^{4+} and V^{5+} below the structural transition at $T_c = 34K$, which clearly indicates that the transition may be driven by charge ordering (CO). In order to probe the rich electronic structure of NaV$_2$O$_5$ specific heat measurements and optical measurements have been performed in magnetic field[3−5]. According to the standard theory, the magnetic field dependence of transition temperature T_c of spin-Peierls system obeys the following equation: $\frac{T_c(H)}{T_c(0)} = 1 - \alpha[g\mu_B H/2k_B T_c(0)]^2$, where the prefactor α equals to 0.44 or 0.36 depending on the way interaction effects are taken into account [6,7]. However, the experimental results are rather controversial as regards the value of the prefactor α. By polarized optical reflectance studies one found $0.22 < \alpha < 0.42$ [3]. In contrary, specific-heat measurements in magnetic field up to 16 Tesla gave $\alpha \approx 0.092$, which is much smaller than expected from spin-Peierls theory[4]. Although it is not clear whether the charge ordering precedes or forms simultaneously with the spin-Peierls state, it seems certain that

the physics of charge ordering must be taken into account, thus stimulating the research reported in this paper. The present paper is devoted to the consideration of the effect of the magnetic field on the CO transition temperature in the simplest model which allows for a CO transition due to the competition between kinetic and Coulomb energy, namely, the extended Hubbard model (EHM) with the nearest neighbor Coulomb interaction. To solve this problem we use coherent potential approximation (CPA), a simple but physically meaningful approximation which allows us to study the reentrant CO behavior in EHM under zero magnetic field as done in Refs. 8-9. Although the CPA treatment of the Hubbard model fails in properly describing the coherent propagation of low-energy quasiparticle in doped Mott insulators, it is not crucial in the doping regimes explored in the present paper[10]. This paper is organized as follows. In next section, we describe the model and the formalism, and then in the Sec. 3 we show the results obtained for the $(T - H)$-phase diagram. A brief summary is given in Sec. 4.

2. Model and Formalism

We study the EHM in magnetic field. The Hamiltonian is given by:

$$H = t \sum_{<ij>\sigma} (c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma}) + U\sum_i n_{i\uparrow}n_{i\downarrow} + V \sum_{<ij>} n_i n_j - \frac{1}{2}g\mu_B H \sum_i (n_{i\uparrow} - n_{i\downarrow}),$$

(1)

where $c_{i\sigma}(c_{i\sigma}^+)$ annihilates (creates) an electron with spin σ at site i, $n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$ and $n_i = n_{i\uparrow} + n_{i\downarrow}$. $< ij >$ denotes nearest neighbors, t is the hopping parameter, U and V are on-site and inter-site Coulomb repulsion, respectively. The fourth term in (2.1) is the Zeeman coupling, where H is the applied magnetic field, μ_B is the Bohr magneton, g is the g-factor in the direction of the magnetic field and is taken to be equal 1.98^{11}. As we are interested in charge ordered phase with different occupancies on the nearest neighbor sites, we divide the cubic lattice in two sublattices such that points on one sublattice have only points of the other sublattice as nearest neighbors. The sublattice is denoted by subindex A or B: $c_{i\sigma} = a_{i\sigma}(b_{i\sigma})$ if $i \in A$ ($i \in B$). First, we perform a mean-field decoupling of the V term in (2.1). Then, by employing the alloy-analog approach we get a one-particle Hamiltionian which is of the form:

$$\tilde{H} = \sum_{i\in A} (E_A^+ a_{i\uparrow}^+ a_{i\uparrow} + E_A^- a_{i\downarrow}^+ a_{i\downarrow}) + \sum_{j\in B} (E_B^+ b_{i\uparrow}^+ b_{i\uparrow} + E_B^- b_{i\downarrow}^+ b_{i\downarrow})$$

$$+ t \sum_{<ij>\sigma} (a_{i\sigma}^+ b_{j\sigma} + b_{j\sigma}^+ a_{i\sigma}) - 3VNn_A n_B,$$

(2)

$$E^{\pm}_{A/B,\sigma} = \begin{cases} 6Vn_{B/A} \mp h & \text{with probability} \quad 1 - n^{\mp}_{A/B,-\sigma}\,, \\ 6Vn_{B/A} \mp h + U & \text{with probability} \quad n^{\mp}_{A/B,-\sigma}\,. \end{cases} \tag{3}$$

Here $n^{\pm}_{A/B}$ is the averaged electron occupation number with spin up (down) in the A/B-sublattice, $n_{A/B} = n^{+}_{A/B} + n^{-}_{A/B}$, N is the number of sites in the lattice and $h = \frac{1}{2}g\mu_B H$. In CPA the averaged local Green functions for A/B-sublattice $\bar{G}_{A/B}$ then take the form

$$\bar{G}^{\pm}_{A/B}(\omega) = \frac{2}{W^2}\left\{\omega - \Sigma^{\pm}_{B/A}(\omega) - \left[(\omega - \Sigma^{\pm}_{B/A}(\omega))^2 - \frac{\omega - \Sigma^{\pm}_{B/A}(\omega)}{\omega - \Sigma^{\pm}_{A/B}(\omega)}W^2\right]^{1/2}\right\}, \tag{4}$$

where we have employed the semi-elliptic density of states (DOS) for non-interacting electron, $\rho_0(\varepsilon) = \frac{2}{\pi W^2}\sqrt{W^2 - \varepsilon^2}$ with the bandwidth W. The CPA demands that the scattering matrix vanishes on average. This yields expression for self-energy $\Sigma^{\pm}_{A/B}(\omega)$ of the form

$$\Sigma^{\pm}_{A/B}(\omega) = \bar{E}^{\pm}_{A/B} - (6Vn_{B/A} - \Sigma^{\pm}_{A/B}(\omega))\bar{G}^{\pm}_{A/B}(\omega)(6Vn_{B/A} + U - \Sigma^{\pm}_{A/B}(\omega))\,, \tag{5}$$

where $\bar{E}^{\pm}_{A/B} = 6Vn_{B/A} \mp h + Un^{\mp}_{A/B}$. From Eqs. (2.4)-(2.5), it is easy to obtain a system of equations for $\bar{G}^{+}_{A/B}$ and $\bar{G}^{-}_{A/B}$. For arbitrary value of electron density n we denote $n_{A/B} = n \pm x$, $n^{\pm}_A = (n_A \pm m_A)/2$, $n^{\pm}_B = (n_B \pm m_B)/2$, where $m_{A/B}$ is the magnetization in A/B-sublattice, then at temperature T we have the following self-consistent system of equations for order parameters x, m_A, m_B and the chemical μ for fixed U, V, T, h and n.

$$n + x = -\frac{1}{\pi}\int_{-\infty}^{+\infty} d\omega f(\omega)\Im(\bar{G}^{+}_A(\omega) + \bar{G}^{-}_A(\omega))\,, \tag{6}$$

$$n - x = -\frac{1}{\pi}\int_{-\infty}^{+\infty} d\omega f(\omega)\Im(\bar{G}^{+}_B(\omega) + \bar{G}^{-}_B(\omega))\,, \tag{7}$$

$$m_A = -\frac{1}{\pi}\int_{-\infty}^{+\infty} d\omega f(\omega)\Im(\bar{G}^{+}_A(\omega) - \bar{G}^{-}_A(\omega))\,, \tag{8}$$

$$m_B = -\frac{1}{\pi}\int_{-\infty}^{+\infty} d\omega f(\omega)\Im(\bar{G}^{+}_B(\omega) - \bar{G}^{-}_B(\omega))\,. \tag{9}$$

Here $f(\omega) = (1 + \exp(\omega - \mu)/k_B T)^{-1}$ is the Fermi function.

We are now interested in the phase boundary between homogeneous ($x = 0$) and charge ordered ($x \neq 0$) phases. In this phase boundary $m_A = m_B \equiv m$ and we make following ansatz: $\bar{G}^{\pm}_A(x = 0, \pm m, \omega) = \bar{G}^{\pm}_B(x = 0, \pm m, \omega) \equiv g(\pm m, \omega)$. We find that the conditions for the onset of CO under a magnetic

field are expressed as

$$n + m = -\frac{2}{\pi} \int_{-\infty}^{+\infty} d\omega f(\omega^-) \Im g(m, \omega) , \tag{10}$$

$$n - m = -\frac{2}{\pi} \int_{-\infty}^{+\infty} d\omega f(\omega^+) \Im g(-m, \omega) , \tag{11}$$

$$1 = -\frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega [f(\omega^-) \Im g'(m, \omega) + f(\omega^+) \Im g'(-m, \omega)], \tag{12}$$

where $\omega^\pm = \omega \pm h$ and $g(\pm m, \omega)$ is a solution with negative imagine part of the cubic equation in the form

$$g^3 - 8\omega g^2 + [16\omega^2 - 4(U^2 - 1)]g - [16\omega + 8U(n - 1 \mp m)] = 0, \tag{13}$$

and $g'(\pm m, \omega)$ are given by $g'(\pm m, \omega) = \frac{\partial \bar{G}^\pm(x, m, \omega)}{\partial x} |_{x=0}$. Hereafter, the bandwidth W is taken to be unity for simplicity. Setting $h = 0$ and $m = 0$ in Eqs. (2.10)-(2.12) we reproduce the CPA equations for the charge ordering in EHM under zero magnetic field in Ref. 8. For fixed temperature T, on-site Coulomb repulsion U, banding filling n and magnetic field H, we have the closed system of equations (2.10)-(2.13) for the critical value V, the chemical potential μ and the magnetization m.

3. Numerical Results and Discussion

We have solved numerically the system of Eqs. (2.10)-(2.13); the results can be summarized as follows:

For small H, magnetic field decreases critical temperature and $T_c(H)$ obeys the following equation

$$\frac{T_c(H)}{T_c(0)} = 1 - \alpha [g\mu_B H / 2k_B T_c(0)]^2 , \tag{3.1}$$

In order to compare our results with experiments, we calculate the prefactor α in the equation (3.1). Fig. 1 shows relative variation of T_c as a function of the scaled magnetic field $g\mu_B H / 2k_B T_c(0)$ for different values of U. The inset in Fig. 1 shows the dependence of the value α on the on-site Coulomb repulsion U for $V = 0.3$ and $n = \frac{1}{2}$. From our calculations for small U the coefficient α decreases with increasing U: for $0.5 \le U \le 1.25$ we find $0.16 \le \alpha \le 0.20$.

As discussed in the introduction, the experimental results are controversial as regards the value of the coefficient α in NaV_2O_5, and there is the difference between the experimental value α and the theoretically predicted one $\alpha \approx 0.36$ for spin-Peierls systems. Although this issue is not fully understood,
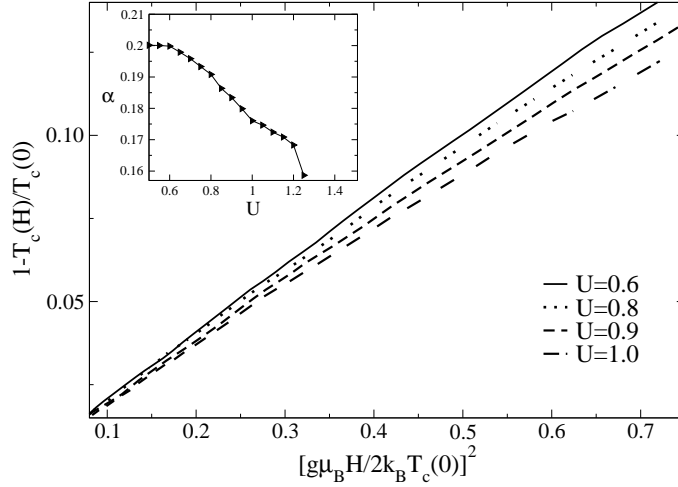
Figure 1: Relative variation of critical temperature as a function of the scale magnetic field for n =0.5, V=0.3. Inset shows the dependence of α on U for n =0.5, V=0.3.

it was argued by Bompardre and coworkers in Ref. 5 that the charge density wave formation is the driving force behind the opening of a spin gap and the "charge" part of the transition is mainly responsible for the $T_c(H)$ dependence, i. e. the physics of charge ordering must be taken into account. Our calculations based on the EHM support this assumption. It is interesting that our results derived from rather simple model are overall in good agreement with experimental measurements.

For intermediate field the critical temperature $T_c(H)$ is not obeyed Eq. (3.1). Furthermore, at various band filling we find that the critical H_c, as a function of temperature T is found to be non-monotous. Consequently, $\frac{dH_c}{dT}$ becomes positive at low temperature, i. e. reentrant CO transition with change of T under fixed H occurs, as can be clearly seen in Fig. 2 . In order to study the reentrant CO behavior in more detail we consider the $(T-H)$ phase diagram for various values of the inter-site and the on-site interactions. The $(T-H)$ phase diagram at quarter filling for various values of the inter-site interaction V is displayed in Fig. 3. Reduction of the CO region with decreasing V is clearly seen. On the other hand, the reentrant charge ordered behavior is found for all values of V in the interval $0.25 < V < 0.4$ with $U = 0.5$. Fig. 4 shows the $(T-H)$ phase diagram at quarter filling for several values
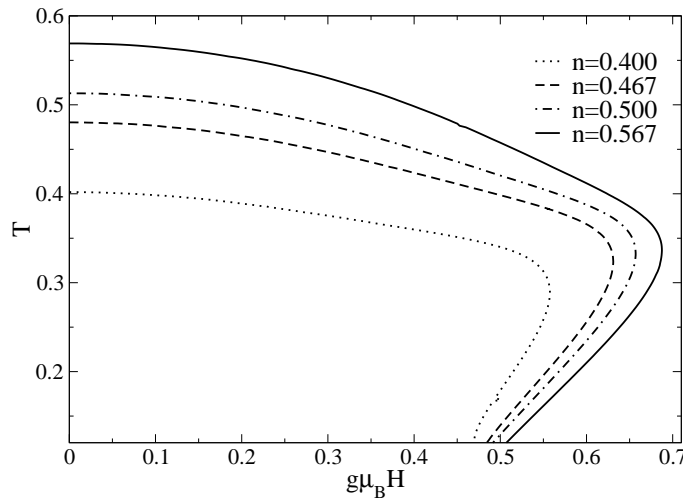
Figure 2: (T-H) phase diagram for U =0.5, V=0.3 at various values of n.

of the on-site interaction U. The reentrant CO is clearly observed within a finite region of h for $U = 0.5, 0.8$. In our calculation the inter-site interaction V is fixed to equal 0.3, for which the reentrant CO is not found under zero magnetic field $H = 0$ for all above values of U. The fact that reentrant CO occurs under a magnetic field for values of V, for which reentrant CO is not observed without magnetic field is not surprised, since application of magnetic field causes the destruction of the charge ordering and at low temperature the transition field may decrease with decreasing temperature due to higher spin entropy of the charge ordered state[11,12]. It is worthy to note that recently a melting of the CO state on decreasing the temperature, i.e., reentrant behavior, has been found in manganites both without[14−17] and under a magnetic field[12,18−20]. On the theoretical side, to our knowledge, only a few studies of the reentrant CO in manganites exits[8,9,13,21−24]. Actually we notice that except Ref. 24, most authors adopted the EHM with the intersite Coulomb interaction as the driving force for CO. Although the EHM likely lacks some important physical infredients for a suitable description of the manganites, the theoretical investigations, based on the EHM, have given a rather reasonable agreement with the experimental results[17] on the reentrant CO in mangannites. However, in order to quantitatively explain the experimental finding, it should take a more realistic model including the double-exchange mechanism,
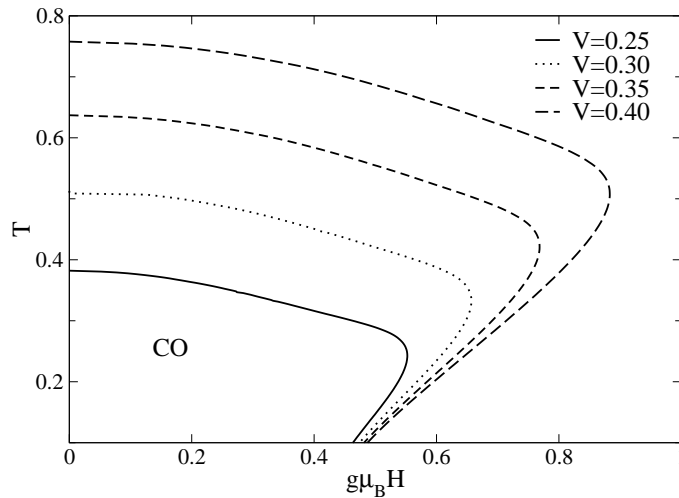
Figure 3: (T-H) phase diagram at quarter filling for U =0.5 and several values of V.

intersite Coulomb interaction and electron-phonon coupling.

4. Conclusions

In this paper we have applied the CPA to study the charge ordering in the extended Hubbard model under a magnetic field. Various phase diagrams in the plane of T and H have shown and discussed. For small H we find that the relative variation of critical temperature is quadratic with the coefficient α smaller than the one for conventional spin-Peierls systems. For small U the coefficient α decreases with increasing U and for $0.5 \leq U \leq 1.25$ we obtained $0.16 \leq \alpha \leq 0.2$. For intermediate field, we find a parameter region of V where the model shows reentrant behavior in $(T - H)$ phase diagram. A melting of the CO on decreasing T under fixed H can be explained in terms of the higher spin entropy of charge ordered state. The calculation presented here can also be improved by including the polaron effect. This is left for future work.
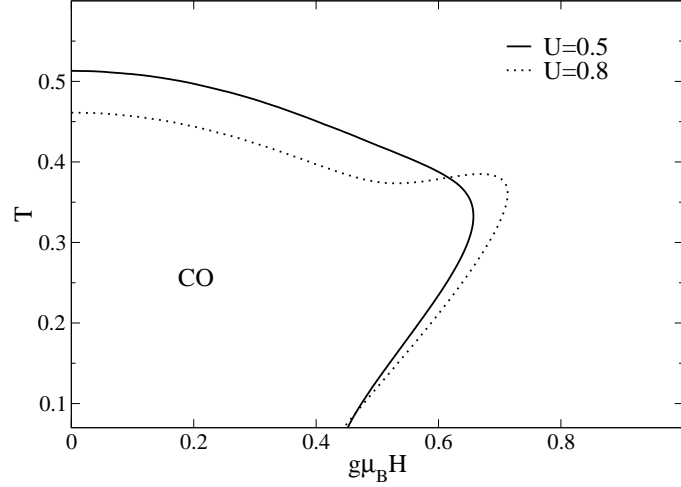
Acknowledgments

Figure 4: (T-H) phase diagram at quarter filling for V=0.3 and different values of U.

References

1. M. Isobe and Y. Veda, J. Phys. Soc. Jpn. **65**, 1178 (1996).

2. T. Ohama et al., Phys. Rev. **B59**, 3299 (1999).

3. V. C. Long et al., Phys. Rev. **B60**, 15721 (1999).

4. W. Schnelle, Yu. Grin and R. K. Kremer, Phys. Rev. **B59**, 73 (1999).

5. S. G. Bompardre et al., Phys. Rev. **B61**, R 13321 (2000).

6. L. N. Bulaevskii, A. I. Buzdin, and D. I. Khomskii, Solid State Commun. **27**, 5 (1978).

7. M. C. Cross, Phys. Rev. **B20**, 4606 (1979).

8. Hoang Anh Tuan, Mod. Phys. Lett. **B15**, 1217 (2001).

9. A. T. Hoang and P. Thalmeier, J. Phys.: Cond. Mat. **14,** 6639 (2002).

10. The authors are grateful to the referee for pointing out this physical issue.

11. Ogawa et al., J. Phys. Soc. Jpn. **55**, 2129 (1986).

12. M. Tokunaga et al., Phys. Rev. **B57**, 5259 (1998).

13. R. Pietig, R. Bulla and S. Blawid, Phys. Rev. Lett. **82**, 4046 (1999).

14. T. Kimura et al., Phys. Rev. Lett. **79**, 3720 (1997).

15. T. Chatterji et al., Phys. Rev. **B61**, 570 (2000).

16. J. Q. Li et al., Phys. Rev. **B64**, 174413 (2001).

17. J. Dho, et al., J. Phys. Cond. Mat. **13,** 3655 (2001).

18. Y. Tomioka et al., Phys. Rev. **B53**, R1689 (1996).

19. M. Prellier et al., Phys. Rev. **B62**, R16337 (2000).

20. E. R. Buzin et al., Appl. Phys. Lett. **79**, 647 (2001).

21. Q. Yuan and P. Thalmeier, Phys. Rev. Lett. **83**, 3502 (1999).

22. C. S. Hellberg, J. Appl. Phys. **89**, 6627 (2001).

23. D. Khomskii, Physica **B280**, 325 (2000).

24. Q. Yuan and T. Kopp, Phys. Rev. **B65**, 174423 (2002).